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by Carl F. Monnin and George M. Prok

Lewis Research Center

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SUMMARY

Excitation and ionization cross sections for electron scattering in metastable atomic hydrogen were calculated by the Born approximation and by the semiclassical theory of Gryzinski. The transitions investigated were excitations from the 2s level to $n = 3, 4$ and ionization. The energy range of the incident electron was from the threshold to 400 electron volts. In the Gryzinski theory the atomic electrons may be assumed to have a distribution of velocities or a single, average velocity. In this report, excitation cross sections calculated with the use of both assumptions are compared with the results of the Born approximation. The cross section resulting from the velocity distribution agreed better with the Born approximation than with the cross section resulting from the average value of the velocity. Since no experimental results are available, the Born approximation above 200 electron volts is assumed correct. The shapes of the Gryzinski-cross-section curves are similar to those for the Born approximation over the energy range investigated.

INTRODUCTION

Many investigators have determined excitation and ionization cross sections for electron impact in atomic hydrogen (refs. 1 to 14). Most of the theoretical and experimental work has been the determination of cross sections for transitions from the ground state of hydrogen (refs. 1 to 10). Cross sections for electron impact in excited atomic hydrogen have been determined by the Born approximation (refs. 11 to 14). References 11 to 14, however, either do not calculate the cross sections of interest or do not carry them to as high an incident energy as they are carried in this report.

The lifetime of the metastable 2s state, in the absence of collisional and electric field quenching, is about 2.4 milliseconds (refs. 15 and 16). Because of this relatively long lifetime, a significant concentration of metastable hydrogen could exist under certain circumstances. Hence, there is a need for cross sections from the 2s level. The object of this report was to calculate excitation cross sections of atomic hydrogen from the 2s to the $n = 3, 4$ levels and to ionization.

The Born approximation and Gryzinski theory were used to calculate inelastic scattering cross sections. The Born approximation was used because it is known to give correct cross sections for high-energy incident electrons; the Gryzinski theory was used because of its easy calculation and because of its past agreement for cross sections from the ground state (ref. 10).

In the Gryzinski model the $s \rightarrow s$ transitions are assumed to take place by electron exchange (ref. 17). All other transitions are assumed to take place by an excitation process. Gryzinski developed two relations for excitation cross sections (refs. 17 and 18). Assuming that the atomic electron has a distribution of velocities leads to a relation with $(\ln E_2)/E_2$ behavior at high energies, while assuming that the atomic electron has a constant average velocity leads to $1/E_2$ behavior, where E_2 is the energy of the incident electron.

The cross sections given by the Born approximation and by the Gryzinski theory are compared in the energy range of threshold to 400 electron volts. In addition, a comparison is made between the two excitation cross sections given by Gryzinski.

THEORY OF SEMICLASSICAL (GRYZINSKI) METHOD

Using classical mechanics, Gryzinski developed a theory giving excitation (refs. 17 and 18) and exchange (ref. 17) cross sections. Gryzinski assumed that $s \rightarrow s$ transitions take place only by the exchange process. The exchange cross section is given by equation (69) of reference 17:

$$Q_e(U_n) = \frac{\sigma_o}{U_n^2} \frac{U_{n+1} - U_n}{U_n} g_e\left(\frac{U_i}{U_n}; \frac{U_i}{U_{n+1}}; \frac{E_2}{U_n}\right) \tag{1}$$

where

$$g_e\left(\frac{U_i}{U_n}; \frac{U_i}{U_{n+1}}; \frac{E_2}{U_n}\right) = \left[\frac{U_n^2}{(E_2 + U_i)(E_2 + U_i - U_n)}\right] \begin{cases} \dfrac{U_n}{E_2 + U_i - U_{n+1}} & \text{if } U_{n+1} \leq E_2 \\[2ex] \dfrac{U_n}{U_i} \dfrac{E_2 - U_n}{U_{n+1} - U_n} & \text{if } U_{n+1} \geq E_2 \end{cases} \tag{2}$$

and

$$\sigma_o = 6.51\times10^{-14}\ (\mathrm{cm}^2)(\mathrm{eV}^2) \tag{3}$$

(A list of symbols is given in appendix A.)

All transitions other than s → s transitions are assumed to take place by an excitation process. In reference 18 Gryzinski assumed that the velocities of the bound electron have some mean value. In reference 17 this assumption is not made, and the target electron has a velocity distribution. The assumption of an average value for velocity of the target electron leads to the excitation cross section given by equation (26) of reference 18:

$$Q(U_n) = \frac{\sigma_o}{U_n^2} g_j\left(\frac{E_2}{U_n}; \frac{E_1}{U_n}\right) \tag{4}$$

where

$$g_j\left(\frac{E_2}{U_n}; \frac{E_1}{U_n}\right) = \left(\frac{E_2}{E_1 + E_2}\right)^{3/2}$$
$$\times\begin{cases} \left[\dfrac{2}{3}\dfrac{E_1}{E_2} + \dfrac{U_n}{E_2}\left(1 - \dfrac{E_1}{E_2}\right) - \left(\dfrac{U_n}{E_2}\right)^2\right] & \text{if } U_n + E_1 \leq E_2 \\ \dfrac{2}{3}\left[\dfrac{E_1}{E_2} + \dfrac{U_n}{E_2}\left(1 - \dfrac{E_1}{E_2}\right) - \left(\dfrac{U_n}{E_2}\right)^2\right]\left[\left(1+\dfrac{U_n}{E_1}\right)\left(1-\dfrac{U_n}{E_2}\right)\right]^{1/2} & \text{if } U_n + E_1 \geq E_2 \end{cases} \tag{5}$$

Averaging the excitation cross section over the velocity distribution of the target electron leads to the form in equation (7) of reference 17:

$$g_j\left(\frac{E_2}{U_n}; \frac{E_1}{U_n}\right) = \frac{E_1}{E_2}\left(\frac{E_2}{E_1 + E_2}\right)^{3/2}$$
$$\times\left\{\frac{U_n}{E_1} + \frac{2}{3}\left(1 - \frac{U_n}{2E_2}\right)\ln\left[2.7 + \left(\frac{E_2 - U_n}{E_1}\right)^{1/2}\right]\right\}\left(1 - \frac{U_n}{E_2}\right)^{1+[E_1/(E_1+U_n)]} \tag{6}$$

In equations (1) to (6) U_n and U_{n+1} are the energies of the n and the n + 1 levels above the energy of the 2s level. The ionization potential is U_i, and E_1 and E_2 are the kinetic energies of the bound and the incident electrons, respectively.

The excitation cross section $Q(U_n)$ is proportional to the probability that the incident electron will lose an amount of energy greater than or equal to the energy difference between level n and the initial (2s) level. The cross section for a given transition to level n is given by

$$Q(U_n;\ U_{n+1}) = Q(U_n) - Q(U_{n+1}) \tag{7}$$

As was pointed out in reference 10, the Gryzinski excitation cross section is for a transition to a principal quantum level and not to the individual sublevels. The Born approximation cross sections to all the sublevels of a principal quantum level, with the exception of the s sublevel, must therefore be summed for comparison with the Gryzinski excitation cross section.

THEORY OF BORN APPROXIMATION

Excitation Cross Section

The first Born approximation is sufficient to determine the cross section for the excitation or ionization of an atom by a fast electron ($v_e >> e^2/h$). The differential cross section for excitation from the 2s level to a higher excited level n with momentum change between K and K + dK is given by

$$I_{ex}(K)dK = \frac{8\pi^3 m_e^2}{h^4} \frac{K\,dK}{k^2} \left| \iint V(\vec{r}, \vec{R}) \exp(i\vec{K} \cdot \vec{R}) \psi_{200}(\vec{r}) \psi^*_{nlm}(\vec{r}) d\tau_r\, d\tau_R \right|^2 \tag{8}$$

where the momentum change is given by

$$\vec{K} = k\hat{y}_0 - k'\hat{y}_1 \tag{9}$$

in which $(kh/2\pi)\hat{y}_0$ and $(k'h/2\pi)\hat{y}_1$ are the initial and the final momentum vectors of the scattered electron, respectively. The wave functions of the 2s level and the higher excited state are $\psi_{200}(\vec{r})$ and $\psi_{nlm}(\vec{r})$, respectively. The potential $V(\vec{r}, \vec{R})$ is the Coulomb potential between the incident electron and the atom. The differential volume elements of the atomic and the incident electrons are $d\tau_r$ and $d\tau_R$, respectively.

The integration of equation (8) is performed in appendix B of this report for a Coulomb potential by using the well-known hydrogen wave functions. The results of the integration are

$$I_{ex}(K)dK = 2^{8l+18} \frac{m_e^2 e^4 \pi^5 n^2}{h^4} (Kna_0)^{2l} (2l + 1) \frac{(n - l - 1)!}{(n + l)!} \frac{\left[(l + 1)!\right]^2}{\left[(n + 2)^2 + 16\zeta^2\right]^{2l+4}} G^2 \frac{dK}{K^3 k^2} \tag{10}$$

where

$$\begin{aligned} G \equiv {} & (nl + n - 1)C_{n-l-1}^{l+2}(X)\epsilon^{n-l-1} - 2n(l + 1)C_{n-l-2}^{l+2}(X)\epsilon^{n-l-2} \\ & + (nl + n + 1)C_{n-l-3}^{l+2}(X)\epsilon^{n-l-3} - \frac{2^4\zeta^2 n(l + 2)}{\left[(n + 2)^2 + 16\zeta^2\right]} \\ & \times \left[C_{n-l-1}^{l+3}(X)\epsilon^{n-l-1} - 4C_{n-l-2}^{l+3}(X)\epsilon^{n-l-2} + 6C_{n-l-3}^{l+3}(X)\epsilon^{n-l-3} \right. \\ & \left. -4C_{n-l-4}^{l+3}(X)\epsilon^{n-l-4} + C_{n-l-5}^{l+3}(X)\epsilon^{n-l-5}\right] \end{aligned} \tag{11}$$

$$X \equiv (n^2 - 4 + 16\zeta^2)\left\{\left[(n + 2)^2 + 16\zeta^2\right]\left[(n - 2)^2 + 16\zeta^2\right]\right\}^{-1/2} \tag{12}$$

$$\epsilon^2 \equiv \frac{\left[(n - 2)^2 + 16\zeta^2\right]}{\left[(n + 2)^2 + 16\zeta^2\right]} \tag{13}$$

$$\zeta \equiv \frac{Kna_0}{2} \tag{14}$$

The functions $C_s^t(X)$ are the Gegenbauer polynomials defined by the generating function

$$\sum_{s=0}^{\infty} C_s^t(X)u^s \equiv \left(1 - 2uX + u^2\right)^{-t} \tag{15}$$

If the coefficients of all the Gegenbauer polynomials with a superscript of $l + 2$ in equation (5) of Boyd (ref. 12) change sign, the results are the same as equation (10) of this report. This fact can be demonstrated by making the sign change and performing algebraic manipulation with the use of the recursion formulas for the Gegenbauer polynomials. Although equation (5) of reference 12 is squared, the cross terms will retain the incorrect sign. Boyd does not present numerical results with this method; he does present results based on the use of parabolic coordinates to discrete principal quantum levels. The numerical results of reference 12 agree well with the equivalent results given herein.

The total cross section of a transition can be obtained by integrating over the allowed momentum change:

$$Q_{ex}(K) = \int_{K_{min}}^{K_{max}} I_{ex}(K)dK \tag{16}$$

where

$$K_{max} = k + k'$$

and

$$K_{min} = k - k'$$

Ionization Cross Section

The differential cross section for ionization from the 2s level is given by

$$I_{\kappa}\, d\kappa\, d\sigma\, d\omega = \frac{4\pi^2 m_e^2}{h^4} \frac{k'}{k} \left| \iint V(\vec{r}, \vec{R}) \exp\left[i(k\hat{y}_0 - k'\hat{y}_1) \cdot \vec{R}\right] \psi_{200}(\vec{r}) \psi_{\kappa}^*(\vec{r}) d\tau_r\, d\tau_R \right|^2 d\kappa\, d\sigma\, d\omega \tag{17}$$

where $\vec{\kappa}$ is the momentum of the ejected electron and $\psi_{\kappa}^*(\vec{r})$ is the Coulomb wave function of the ejected electron. The solid angle into which the target electron is ejected is $d\sigma$, and the solid angle into which the incident electron is scattered is $d\omega$.

The integration of equation (17) is given in appendix C; the result of the integration is

$$I_\kappa \, d\kappa \, d\sigma \, d\omega = I(K, \kappa) dK \, d\kappa = \frac{2^8 \pi \kappa}{15 k^2 K a_0^8} \frac{\exp\left(-\frac{2\mu}{\kappa} \arctan \frac{\mu\kappa}{\frac{\mu^2}{4} + K^2 - \kappa^2}\right) A \, dK \, d\kappa}{\left[1 - \exp\left(-\frac{2\pi}{\kappa a_0}\right)\right]\left\{\left[\frac{\mu^2}{4} + (K + \kappa)^2\right]\left[\frac{\mu^2}{4} + (K - \kappa)^2\right]\right\}^5} \tag{18}$$

where

$$A \equiv \frac{5}{256} \mu^{10} + \frac{\mu^8}{256} (47K^2 + 85\kappa^2) + \frac{\mu^6}{16} (25K^4 + 35\kappa^4)$$

$$+ \frac{\mu^4}{8} (205K^6 - 155K^4\kappa^2 - 41K^2\kappa^4 + 55\kappa^6)$$

$$- 10\mu^2\left(K^2 - \kappa^2\right)^2 (4K^4 - K^2\kappa^2 - \kappa^4) + 5\left(K^2 - \kappa^2\right)^4 (3K^2 + \kappa^2) \tag{19}$$

and

$$\mu \equiv \frac{1}{a_0} \tag{20}$$

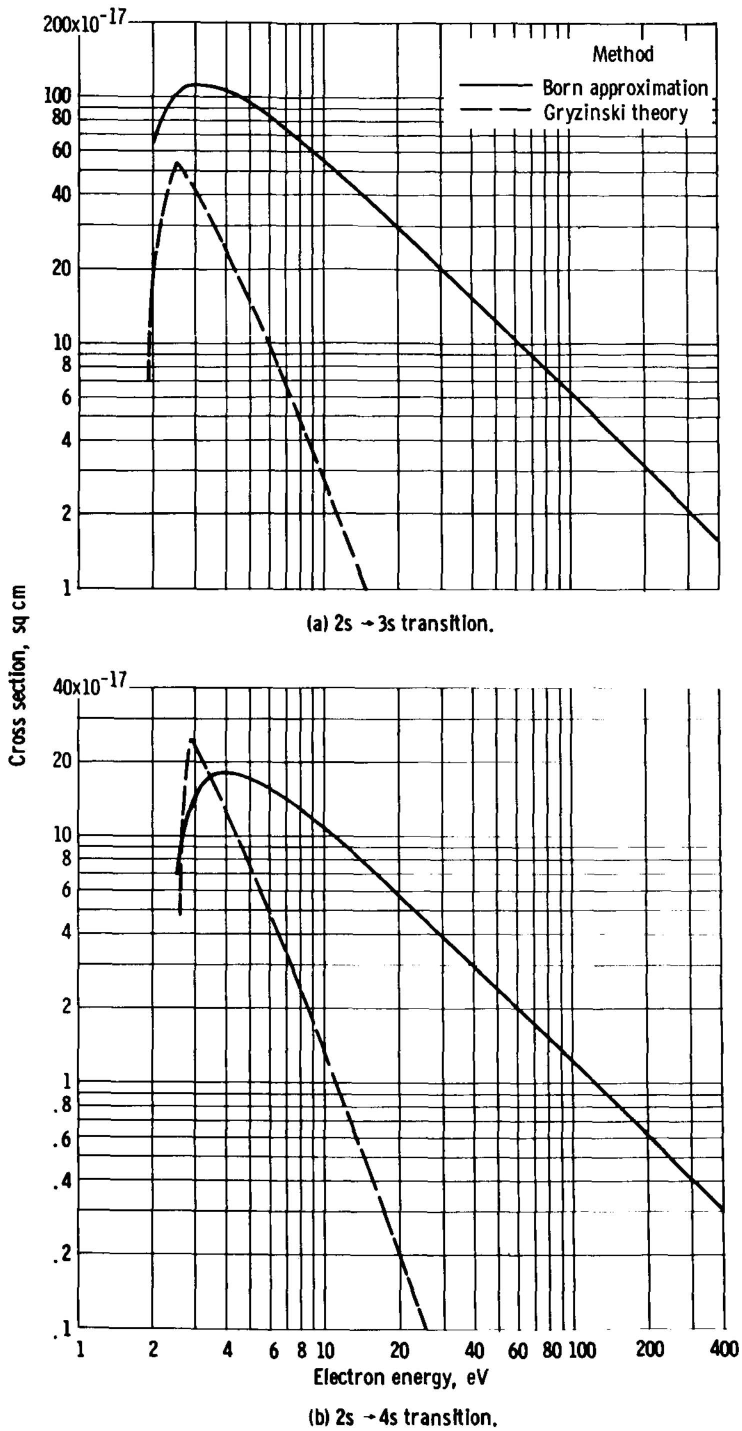
Thus, the total ionization cross section becomes

$$Q_{ion}(K, \kappa) = \int_0^{\kappa_{max}} \int_{K_{min}}^{K_{max}} I(K, \kappa) dK \, d\kappa \tag{21}$$

These results follow from a method given in reference 9 for ionization of atomic hydrogen in the ground state.

RESULTS AND DISCUSSION

The calculated results of the $2s \rightarrow ns$ transitions are presented in figure 1. The Gryzinski cross sections are much sharper than the Born cross sections and are



(b) 2s → 4s transition.

Figure 1. - Atomic hydrogen cross section for 2s → ns transitions.

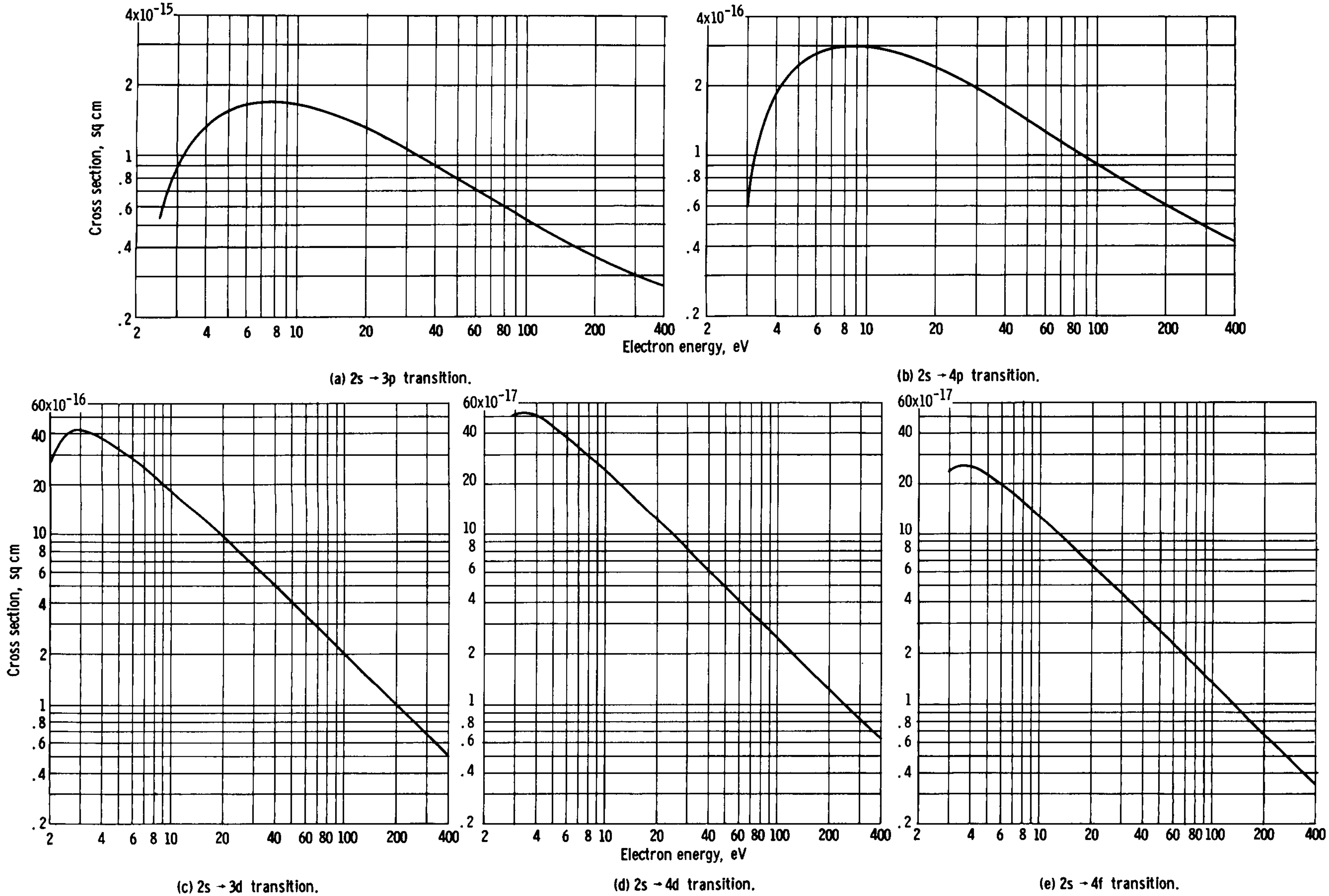


Figure 2. - Born approximation of atomic hydrogen cross section for 2s → nl transitions.

negligible at incident electron energies above 25 electron volts. Because of the sharpness of the peak and the size of the steps used in the numerical analysis, the maximum of the cross section may be higher than indicated in figure 1.

The Born approximation cross sections for the 2s → np, 2s → nd, and 2s → 4f transitions are shown in figure 2. The classical theory of Gryzinski, with and without the velocity distribution, was used to obtain composite cross sections for transitions from the 2s level to higher excited principal quantum levels. The Born approximation cross sections for all the sublevels of a principal quantum level are summed to obtain a composite cross section which can be compared with that given by the Gryzinski theory. The composite cross sections are shown in figures 3 and 4 for principal quantum levels 3 and 4, respectively. The Gryzinski theory with the velocity distribution agrees better with the Born approximation than does the Gryzinski theory which uses an average value for the velocity.

In figure 5, the 2s → ionization cross section is presented for the Born approximation and for the classical theory of Gryzinski with and without the velocity distribution. Again, the cross section resulting from the use of the velocity distribution agrees better with the Born approximation. The cross section resulting from the distribution crosses the Born approximation at about 20 and again at about 200 electron volts and lies between the cross sections given by the other theories.

The Born approximation formula for the 2s → ionization transition agrees with that of Burhop (ref. 11). Boyd (ref. 12), Swan (ref. 13), and Mandl (ref. 14) have also derived the ionization cross section from the 2s level. Because there are misprints in

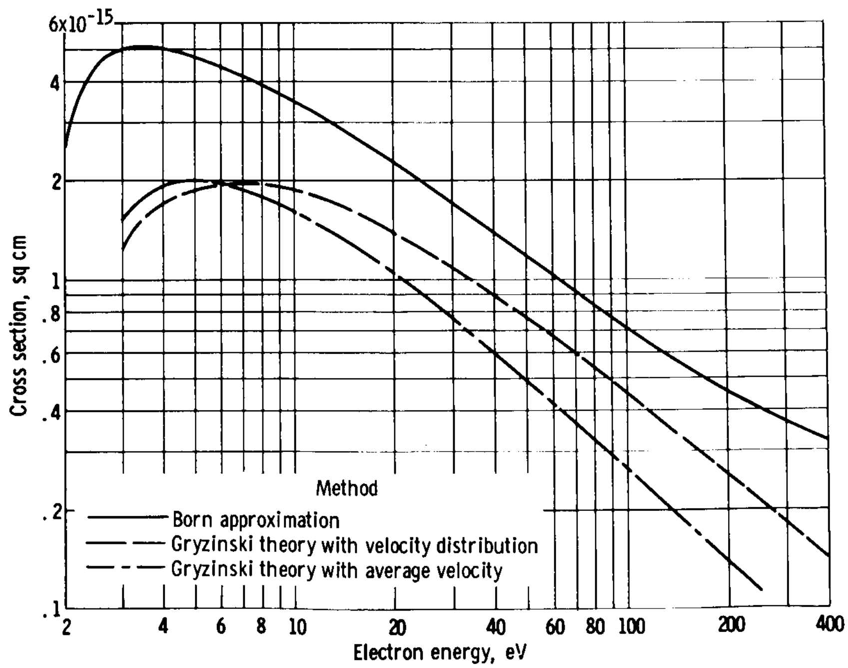


Figure 3. - Atomic hydrogen cross section for 2s → (3p + 3d) transition.

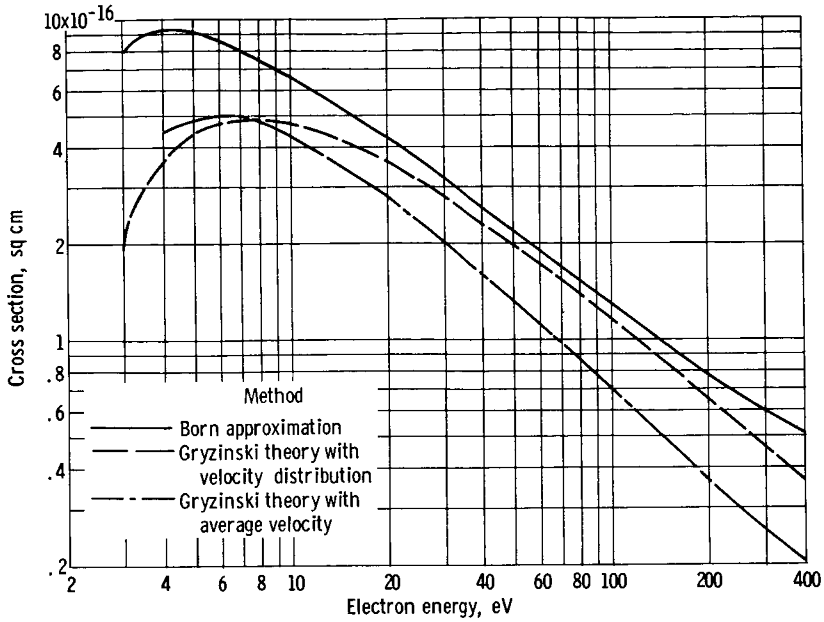


Figure 4. - Atomic hydrogen cross section for 2s → (4p + 4d + 4f) transition.

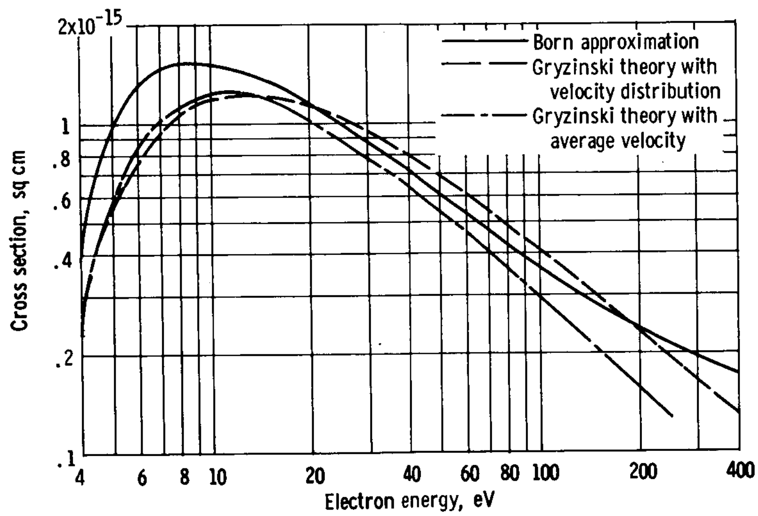


Figure 5. - Atomic hydrogen cross section for 2s → ionization transition.

these papers, the formula was rederived herein. None of these authors present numerical calculations for the 2s → ionization transition.

CONCLUDING REMARKS

The Gryzinski exchange theory produces cross sections that peak sharply at low energies and become negligible above 25 electron volts. The Born approximation gives results that are higher than those given by the Gryzinski theory for energies in the range of a few electron volts above onset energy to 400 electron volts.

For excitation cross sections, better agreement with the Born approximation is obtained when a velocity distribution is assumed for the target electrons in the Gryzinski theory. At high energies this approximation leads to $(\ln E_2)/E_2$ behavior, compared with the $1/E_2$ behavior which results from assuming an average velocity.

Similar results hold for the ionization of the 2s level. In the high-energy range, where the theories should be valid, the excitation-cross-section formula gives better results when a velocity distribution of the target electron is used than when an average value of velocity is used. The main difference is that the Gryzinski theory with the velocity distribution yields results above those of the Born approximation in the intermediate energy range between 20 and 200 electron volts.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, October 26, 1966,
129-01-05-09-22.

APPENDIX A

SYMBOLS

A defined by eq. (19)

a_0 Bohr radius, cm

$C_s^t(X)$ Gegenbauer polynomial defined by eq. (15)

E_κ kinetic energy of ejected electron, eV

E_1 kinetic energy of atomic electron, eV

E_2 kinetic energy of incident electron, eV

$\mathcal{E}_m$ Neumann number (1 for $m = 0$; 2 for $m \neq 0$)

e electronic charge, esu

$_pF_q$ hypergeometric function, Pochhammer notation

G defined by eq. (11)

g_e defined by eq. (2)

g_j defined by eqs. (5) and (6)

h Planck's constant, erg-sec

I defined by eq. (C33)

$I_{ex}(K)$ Born's differential excitation cross section, cm^2

I_κ Born's differential ionization cross section, cm^2

$J_p(x)$ Bessel function of order p and argument x

K magnitude of momentum change for exciting collision, cm^{-1}

k wave number of incident electron, cm^{-1}

k' wave number of scattered electron in exciting collision, cm^{-1}

k_κ wave number of ejected electron in ionizing collision, cm^{-1}

L_{n+l}^{2l+1} Laguerre polynomial

l orbital angular momentum quantum number

m magnetic quantum number

m_e mass of electron, g

N_{nlm} normalizing factor

n principal quantum number

$P_l^m(x)$ Legendre polynomial

$Q(U_n)$ excitation cross section, Gryzinski, cm^2

$Q_e(U_n)$ exchange cross section, Gryzinski, cm^2

Q_{ex} excitation cross section, Born approximation, cm^2

Q_{ion} ionization cross section, Born approximation, cm^2

R magnitude of radius vector of incident electron, cm

r, θ, φ spherical coordinates of atomic electron

s, p, d, f	energy levels for $l = 0, 1, 2, 3$, respectively
U_i	ionization potential, eV
U_n	energy of level n, eV
$V(\vec{r}, \vec{R})$	Coulomb potential between electron and atom, $(esu^2)(cm^{-1})$
v_e	speed of incident electron, $(cm)(sec^{-1})$
X	defined by eq. (12)
$\hat{y}_\kappa$	unit vector in direction of ejected electron
$\hat{y}_0$	unit vector in direction of incident electron
$\hat{y}_1$	unit vector in direction of scattered electron
$\Gamma(x)$	gamma function of argument x
$\delta, \Theta, \chi, \psi$	angles defined in fig. 6
ϵ	defined in eq. (13)
ζ	$Kna_0/2$
κ	magnitude of momentum of ejected electron, cm^{-1}
μ	$1/a_0$, cm^{-1}
σ_o	$\pi e^4 z^2$ for incident particle, $(cm^2)(eV^2)$
$d\sigma$	solid angle into which target electron is ejected
$d\tau_R$	differential volume element in coordinate space of bound electron
$d\tau_r$	differential volume element in coordinate space of incident electron
$\psi_{nlm}(\vec{r})$	wave function
$\psi_\kappa^*(\vec{r})$	Coulomb wave function
$d\omega$	solid angle into which incident electron is scattered

Superscripts:

$\rightarrow$	vector
*	complex conjugate

APPENDIX B

DERIVATION OF BORN EXCITATION FORMULA

The integral to be evaluated is

$$I_{ex}(K)dK = \frac{8\pi^3 m_e^2}{h^4} \frac{K\,dK}{k^2} \left| \iint V(\vec{r}, \vec{R}) \exp(i\vec{K} \cdot \vec{R}) \psi_{200}(\vec{r}) \psi^*_{nlm}(\vec{r}) d\tau_r \, d\tau_R \right|^2 \tag{8}$$

where the potential $V(\vec{r}, \vec{R})$ is the Coulomb potential between the incident electron and the atom. Because of the orthogonality of the atomic wave functions, the Coulomb interaction between the incident electron and the atomic nucleus vanishes.

Substituting the potential and the wave functions into equation (8) gives

$$I_{ex}(K)dK = \frac{8\pi^3 m_e^2}{h^4} \frac{K\,dK}{k^2}$$

$$\times \left| 2N_{200}N_{nlm}e^2 \iint \frac{\exp(i\vec{K} \cdot \vec{R})}{|\vec{r} - \vec{R}|} \left(2 - \frac{r}{a_0}\right) \exp\left(\frac{-r}{2a_0}\right) \left(\frac{2r}{na_0}\right)^l P_l^m(\cos\theta) \right.$$

$$\left. \times \exp(\pm im\varphi) \exp\left(\frac{-r}{na_0}\right) L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right) d\tau_r \, d\tau_R \right|^2 \tag{B1}$$

where

$$N_{nlm}^2 = \frac{(2l + 1)}{4\pi} \frac{(l - m)!}{(l + m)!} \left(\frac{2}{na_0}\right)^3 \frac{(n - l - 1)!}{2n\left[(n + l)!\right]^3} \tag{B2}$$

Integration over the coordinates of the incident electron by the usual method (ref. 19, p. 163) gives

$$\int \frac{e^2}{|\vec{r} - \vec{R}|} \exp(i\vec{K} \cdot \vec{R}) d\tau_R = \frac{4\pi}{K^2} e^2 \exp(i\vec{K} \cdot \vec{r}) \tag{B3}$$

Expressing the coordinates of the atomic electron as spherical coordinates and substituting equation (B3) into equation (B1) give

$$I_{ex}(K)dK = \frac{8\pi^3 m_e^2}{h^4}\frac{K\,dK}{k^2}\left|2N_{200}N_{nlm}\frac{e^2 4\pi}{K^2}\int_0^\infty\int_0^\pi\int_0^{2\pi}\exp(iKr\cos\theta)\left(2-\frac{r}{a_0}\right)\exp\left(\frac{-r}{2a_0}\right)\right.$$

$$\left.\times\left(\frac{2r}{na_0}\right)^l P_l^m(\cos\theta)\exp(\pm im\varphi)\exp\left(\frac{-r}{na_0}\right)L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)r^2\sin\theta\,d\varphi\,d\theta\,dr\right|^2 \tag{B4}$$

The integral over φ is

$$I_\varphi = \int_0^{2\pi}\exp(\pm im\varphi)d\varphi = \begin{cases}2\pi & \text{for } m = 0\\ 0 & \text{for } m \neq 0\end{cases} \tag{B5}$$

Because $P_l^0 \equiv P_l$, the integral over θ is given by

$$I_\theta = \int_0^\pi \exp(iKr\cos\theta)P_l(\cos\theta)\sin\theta\,d\theta \tag{B6}$$

From reference 20 (p. 77),

$$P_l(\cos\theta) = C_l^{1/2}(\cos\theta) \tag{B7}$$

where $C_l^{1/2}(\cos\theta)$ is a Gegenbauer polynomial. From reference 20 (p. 77),

$$I_\theta = \sqrt{2\pi}\, i^l \frac{J_{l+(1/2)}(Kr)}{\sqrt{Kr}} \tag{B8}$$

The integral over r becomes

$$I_r = \int_0^\infty \frac{J_{l+(1/2)}(Kr)}{\sqrt{Kr}}\left(2-\frac{r}{a_0}\right)\exp\left(\frac{-r}{2a_0}\right)\left(\frac{2r}{na_0}\right)^l\exp\left(\frac{-r}{na_0}\right)L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)r^2\,dr \tag{B9}$$

An integral is defined:

$$I(n, l, s) \equiv \alpha \int_0^\infty J_{l+(1/2)}(\xi\zeta)\left(2 - \frac{n}{2}\xi\right)\exp\left[-\frac{\xi}{4}(n+2)\right]\xi^{l+(3/2)}L_{2l+1+s}^{2l+1}(\xi)d\xi \tag{B10}$$

where

$$\alpha \equiv \left(\frac{na_0}{2}\right)^{5/2}\frac{1}{\sqrt{K}} \tag{B11}$$

$$\xi = \frac{2r}{na_0} \tag{B12}$$

$$\zeta = \frac{Kna_0}{2} \tag{B13}$$

and l, n, and s are integral constants. Multiplying equation (B10) by $u^s/(2l + 1 + s)!$ and summing on s yield

$$\sum_{s=0}^{\infty}\frac{I(n, l, s)u^s}{(2l+1+s)!} = \alpha\int_0^\infty\left[\sum_{s=0}^{\infty}L_{2l+1+s}^{2l+1}(\xi)\frac{u^s}{(2l+1+s)!}\right]$$

$$\times J_{l+(1/2)}(\xi\zeta)\left(2 - \frac{n}{2}\xi\right)\exp\left[-\frac{\xi}{4}(n+2)\right]\xi^{l+(3/2)}\,d\xi \tag{B14}$$

The generating function for the Laguerre polynomial as given by Schiff (ref. 19, p. 85) is

$$\sum_{s=0}^{\infty}L_{2l+1+s}^{2l+1}(\xi)\frac{u^s}{(2l+1+s)!} = \frac{-\exp\left[-\xi\left(\frac{u}{1-u}\right)\right]}{(1-u)^{2l+2}} \tag{B15}$$

Combining equations (B14) and (B15) gives

$$\sum_{s=0}^{\infty}\frac{I(n, l, s)u^s}{(2l+1+s)!} = \frac{-\alpha}{(1-u)^{2l+2}}\int_0^\infty J_{l+(1/2)}(\xi\zeta)\left(2 - \frac{n}{2}\xi\right)\exp\left\{\frac{-\xi}{4}\left[\frac{(n+2)-(n-2)u}{1-u}\right]\right\}\xi^{l+(3/2)}\,d\xi \tag{B16}$$

For the particular value $s = n - l - 1$, equations (B9) and (B10) indicate that $I(n, l, n - l - 1) \equiv I_r$; thus I_r may be evaluated by determining the coefficient of u^{n-l-1} on the right side of equation (B16). From reference 20 (p. 32),

$$\int_0^\infty \exp(-a\xi)J_\nu(\xi\zeta)\xi^{\mu-1}\, d\xi = \frac{\left(\frac{\zeta}{2a}\right)^\nu \Gamma(\mu + \nu)}{a^\mu \Gamma(\nu + 1)} \; {}_2F_1\left(\frac{\mu + \nu}{2}, \frac{\mu + \nu + 1}{2}; \nu + 1; -\frac{\zeta^2}{a^2}\right) \tag{B17}$$

By using the following properties of the hypergeometric function (ref. 20)

$${}_2F_1(a,b;\ c;\ z) = {}_2F_1(a,b;\ c + 1;\ z) + \frac{abz}{c(c + 1)}\, {}_2F_1(a + 1,\ b + 1;\ c + 2;\ z) \tag{B18}$$

$${}_2F_1(a,b;\ c;\ d) = {}_2F_1(b,a;\ c;\ d) \tag{B19}$$

and

$${}_2F_1(-n,m;\ m;\ -x) = (1 + x)^n \tag{B20}$$

equation (B16) can be stated in the following form:

$$\sum_{s=0}^{\infty} \frac{I(n,l,s)u^s}{(2l + 1 + s)!} = \frac{\alpha}{(1 - u)^{2l+2}} \left[\frac{2\zeta(1 - u)}{(n + 2) - (n - 2)u}\right]^{l+(1/2)} \frac{(2l + 2)!}{\Gamma\left(l + \frac{3}{2}\right)}$$

$$\times \left[\frac{4(1 - u)}{(n + 2) - (n - 2)u}\right]^{l+(5/2)} \left[-2\left\{1 + \frac{16\zeta^2(1 - u)^2}{[(n + 2) - (n - 2)u]^2}\right\}^{-(l+2)}\right.$$

$$+ \frac{n}{2}(2l + 3)\frac{4(1 - u)}{[(n + 2) - (n - 2)u]}\left(\left\{1 + \frac{16\zeta^2(1 - u)^2}{[(n + 2) - (n - 2)u]^2}\right\}^{-(l+2)}\right.$$

$$\left.\left. - \frac{(2l + 4)}{(2l + 3)} \frac{16\zeta^2(1 - u)^2}{[(n + 2) - (n - 2)u]^2}\left\{1 + \frac{16\zeta^2(1 - u)^2}{[(n + 2) - (n - 2)u]^2}\right\}^{-(l+3)}\right)\right] \tag{B21}$$

Equation (B21) can be written as

$$\sum_{s=0}^{\infty} \frac{I(n, l, s)u^s}{(2l + 1 + s)!} = B(1 - u) \frac{[(n+2) - (n-2)u]}{\left(1 - 2Xv + v^2\right)^{l+2}} + \frac{C(1 - u)^2}{\left(1 - 2Xv + v^2\right)^{l+2}} - \frac{D(1 - u)^4}{\left(1 - 2Xv + v^2\right)^{l+3}} \tag{B22}$$

where

$$v \equiv u\left[\frac{(n - 2)^2 + 16\zeta^2}{(n + 2)^2 + 16\zeta^2}\right]^{1/2} \equiv \epsilon u \tag{B23}$$

$$X \equiv \frac{1}{\epsilon}\left[\frac{n^2 - 4 + 16\zeta^2}{(n + 2)^2 + 16\zeta^2}\right] \tag{B24}$$

$$B \equiv \frac{-\alpha 2^{3l+(13/2)}\zeta^{l+(1/2)}(2l+2)!}{\left[(n + 2)^2 + 16\zeta^2\right]^{l+2}\Gamma\left(l + \frac{3}{2}\right)} \tag{B25}$$

$$C \equiv \frac{\alpha 2^{3l+(13/2)}\zeta^{l+(1/2)}n(2l + 3)!}{\left[(n + 2)^2 + 16\zeta^2\right]^{l+2}\Gamma\left(l + \frac{3}{2}\right)} \tag{B26}$$

$$D \equiv \frac{\alpha 2^{3l+(21/2)}\zeta^{l+(5/2)}n(2l + 2)!(2l + 4)}{\left[(n + 2)^2 + 16\zeta^2\right]^{l+3}\Gamma\left(l + \frac{3}{2}\right)} \tag{B27}$$

Expanding $(1 - 2Xv + v^2)$ in terms of Gegenbauer polynomials, equating coefficients of u, and recalling that $I(n, l, n - l - 1) \equiv I_r$ give

$$I_r = \frac{\alpha 2^{3l+(13/2)} \zeta^{l+(1/2)} (2l+2)!(n+l)!}{\left[(n+2)^2 + 16\zeta^2\right]^{l+2} \Gamma\left(l + \frac{3}{2}\right)} \Bigg\{ 2(nl + n - 1) C_{n-l-1}^{l+2}(X) \epsilon^{n-l-1}$$

$$- 4n(l+1) C_{n-l-2}^{l+2}(X) \epsilon^{n-l-2} + 2(nl + n + 1) C_{n-l-3}^{l+2}(X) \epsilon^{n-l-3}$$

$$- \frac{2^5 \zeta^2 n(l+2)}{\left[(n+2)^2 + 16\zeta^2\right]} \Big[C_{n-l-1}^{l+3}(X) \epsilon^{n-l-1} - 4C_{n-l-2}^{l+3}(X) \epsilon^{n-l-2}$$

$$+ 6C_{n-l-3}^{l+3}(X) \epsilon^{n-l-3} - 4C_{n-l-4}^{l+3}(X) \epsilon^{n-l-4} + C_{n-l-5}^{l+3}(X) \epsilon^{n-l-5} \Big] \Bigg\} \tag{B28}$$

Substituting equations (B5), (B8), and (B28) into equation (6) gives

$$I_{ex}(K)dK = 2^{8l+18} \frac{m_e^2 e^4 \pi^5 n^2}{h^4} (Kna_0)^{2l} (2l+1) \frac{(n-l-1)!}{(n+l)!} \frac{\left[(l+1)!\right]^2}{\left[(n+2)^2 + 16\zeta^2\right]^{2l+4}} G^2 \frac{dK}{K^3 k^2} \tag{10}$$

where

$$G \equiv (nl + n - 1) C_{n-l-1}^{l+2}(X) \epsilon^{n-l-1} - 2n(l+1) C_{n-l-2}^{l+2}(X) \epsilon^{n-l-2}$$

$$+ (nl + n + 1) C_{n-l-3}^{l+2}(X) \epsilon^{n-l-3} - \frac{2^4 \zeta^2 n(l+2)}{\left[(n+2)^2 + 16\zeta^2\right]}$$

$$\times \Big[C_{n-l-1}^{l+3}(X) \epsilon^{n-l-1} - 4C_{n-l-2}^{l+3}(X) \epsilon^{n-l-2} + 6C_{n-l-3}^{l+3}(X) \epsilon^{n-l-3}$$

$$-4C_{n-l-4}^{l+3}(X) \epsilon^{n-l-4} + C_{n-l-5}^{l+3}(X) \epsilon^{n-l-5} \Big] \tag{11}$$

$$X \equiv (n^2 - 4 + 16\zeta^2) \left\{ \left[(n+2)^2 + 16\zeta^2\right] \left[(n-2)^2 + 16\zeta^2\right] \right\}^{-1/2} \tag{12}$$

$$\epsilon^2 \equiv \frac{\left[(n - 2)^2 + 16\zeta^2\right]}{\left[(n + 2)^2 + 16\zeta^2\right]} \tag{13}$$

$$\zeta \equiv \frac{Kna_0}{2} \tag{14}$$

APPENDIX C

DERIVATION OF BORN IONIZATION FORMULA

The integral to be evaluated is

$$I_\kappa \, d\kappa \, d\sigma \, d\omega = \frac{4\pi^2 m_e^2}{h^4} \frac{k'}{k} \left| \iint V(\vec{r}, \vec{R}) \exp\left[i(k\hat{y}_0 - k'\hat{y}_1) \cdot \vec{R}\right] \psi_{200}(\vec{r}) \psi_\kappa^*(\vec{r}) d\tau_r \, d\tau_R \right|^2 d\kappa \, d\sigma \, d\omega \tag{17}$$

where $V(\vec{r}, \vec{R})$ is the Coulomb potential between the incident electron and the atomic electron. The metastable 2s wave function is ψ_{200}, and $\psi_\kappa^*(\vec{r})$ is the Coulomb wave function.

$$\psi_{200}(\vec{r}) = \frac{1}{4\sqrt{2\pi a_0^3}} \left(2 - \frac{r}{a_0}\right) \exp\left(\frac{-r}{2a_0}\right) \tag{C1}$$

$$\psi_\kappa^*(\vec{r}) = \frac{\kappa}{2\pi} \left[\frac{n}{1 - \exp(-2\pi n)}\right]^{1/2} \frac{\exp(i\kappa r)}{\Gamma(1 - in)} \int_0^\infty u^{-in} e^{-u} J_0\left[2(i\kappa\xi' u)^{1/2}\right] du \tag{C2}$$

where

$$\xi' \equiv r(1 + \cos \Theta) \tag{C3}$$

$$\cos \Theta \equiv \cos \theta \cos \psi + \sin \theta \sin \psi \cos(\varphi - \chi) \tag{C4}$$

(The angles χ, Θ, θ, ψ, and φ are shown in fig. 6.)

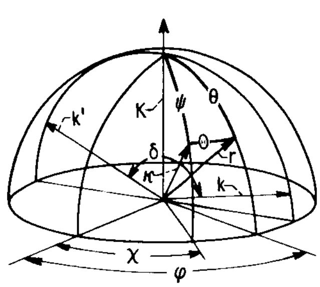


Figure 6. - Directions and angles involved in ionizing collision.

$$n \equiv \frac{1}{\kappa a_0} \tag{C5}$$

The momentum change of the incident electron is defined as

$$\vec{K} \equiv k\hat{y}_0 - k'\hat{y}_1 \tag{C6}$$

and the momentum of the ejected electron is defined as

$$\vec{\kappa} \equiv \sqrt{\frac{8\pi^2 m_e E_\kappa}{h^2}}\,\hat{y}_\kappa \tag{C7}$$

where E_κ is the energy of the atom measured with respect to its ionization limit. The potential is given by

$$V(\vec{r}, \vec{R}) = \frac{e^2}{|\vec{r} - \vec{R}|} \tag{C8}$$

Substituting equations (C1), (C2), (C6), and (C8) into equation (17) gives

$$I_\kappa \, d\kappa \, d\sigma \, d\omega = \alpha \left| \iint \frac{e^2}{|\vec{r} - \vec{R}|} \exp(i\vec{K} \cdot \vec{R}) \left(2 - \frac{r}{a_0}\right) \exp\left(\frac{-r}{2a_0}\right) \exp(i\kappa r) \int_0^\infty u^{-in} \exp(-u) \right.$$

$$\left. \times J_0\left[2(i\kappa\xi' u)^{1/2}\right] du \, d\tau_R \, d\tau_r \right|^2 d\kappa \, d\sigma \, d\omega \tag{C9}$$

where

$$\alpha \equiv \frac{m_e^2}{32\pi a_0^3 h^4 \left[\Gamma(1 - in)\right]^2} \left[\frac{n}{1 - \exp(-2\pi n)}\right] \frac{\kappa^2 k'}{k} \tag{C10}$$

By the usual method (ref. 19, p. 163), integration over the coordinates of the incident electron gives

$$\int \frac{e^2}{|\vec{r} - \vec{R}|} \exp(i\vec{K} \cdot \vec{R}) d\tau_R = \frac{4\pi}{K^2} e^2 \exp(i\vec{K} \cdot \vec{r}) \tag{C11}$$

Equations (C4) and (C11) are substituted into equation (C9), and parabolic coordinates ξ, η, and φ are introduced, where

$$\xi = r(1 + \cos\theta) \tag{C12}$$

and

$$\eta = r(1 - \cos\theta) \tag{C13}$$

Therefore,

$$r = \frac{\xi + \eta}{2} \tag{C14}$$

$$\cos\theta = \frac{\xi - \eta}{2r} \tag{C15}$$

$$\sin\theta = \frac{\sqrt{\xi\eta}}{r} \tag{C16}$$

$$d\tau_r = \frac{(\xi + \eta)}{4}\, d\xi\, d\eta\, d\varphi \tag{C17}$$

From reference 20 (p. 21),

$$J_0\left[2(i\kappa\xi'u)^{1/2}\right] = \sum_{m=0}^{\infty} \varepsilon_m J_m\left\{2\left[i\kappa\xi\left(\cos^2\frac{\psi}{2}\right)u\right]^{1/2}\right\} J_m\left\{2\left[i\kappa\eta\left(\sin^2\frac{\psi}{2}\right)u\right]^{1/2}\right\}\cos m(\pi - \varphi + \chi) \tag{C18}$$

where ε_m is the Neumann number ($\varepsilon_0 = 1$ and $\varepsilon_m = 2$ for $m = 1, 2, 3, \ldots$). Substituting equations (C10) to (C18) into equation (C9) gives

$$I_\kappa\, d\kappa\, d\sigma\, d\omega = \frac{16\pi^2 e^4}{K^4}\,\alpha \left| \int_0^\infty \int_0^\infty \int_0^\infty \int_0^{2\pi} \exp\left(iK\,\frac{\xi - \eta}{2}\right)\left(2 - \frac{\xi + \eta}{2a_0}\right)\exp\left(i\kappa\,\frac{\xi + \eta}{2}\right)u^{-in} \right.$$

$$\times \exp(-u)\exp\left(-\frac{\xi + \eta}{4a_0}\right)\sum_{m=0}^{\infty}\varepsilon_m J_m\left\{2\left[i\kappa\xi\left(\cos^2\frac{\psi}{2}\right)u\right]^{1/2}\right\}$$

$$\left. \times J_m\left\{2\left[i\kappa\eta\left(\sin^2\frac{\psi}{2}\right)u\right]^{1/2}\right\}\cos m(\pi - \varphi + \chi)\,\frac{(\xi+\eta)}{4}\,d\varphi\, d\xi\, d\eta\, du \right|^2 d\kappa\, d\sigma\, d\omega \tag{C19}$$

The integral over φ has the form

$$\int_0^{2\pi} \cos m(\pi - \varphi + \chi)d\varphi = \begin{cases} 2\pi & \text{for } m = 0 \\ 0 & \text{for } m \neq 0 \end{cases} \tag{C20}$$

Combining equations (C19) and (C20) and substituting $\mu \equiv 1/a_0$ give

$$I_\kappa \, d\kappa \, d\sigma \, d\omega = \frac{64\pi^4 e^4}{K^4} \alpha \left| \left(-2 \frac{\partial}{\partial \mu} - 2\mu \frac{\partial^2}{\partial \mu^2} \right) H \right|^2 d\kappa \, d\sigma \, d\omega \tag{C21}$$

where

$$H \equiv \int_0^\infty \int_0^\infty \int_0^\infty \exp\left(iK \frac{\xi - \eta}{2} - \mu \frac{\xi + \eta}{4} + i\kappa \frac{\xi + \eta}{2} - u \right) u^{-in}$$

$$\times J_0 \left\{ 2 \left[i\kappa\xi \left(\cos^2 \frac{\psi}{2} \right) u \right]^{1/2} \right\} J_0 \left\{ 2 \left[i\kappa\eta \left(\sin^2 \frac{\psi}{2} \right) u \right]^{1/2} \right\} d\xi \, d\eta \, du \tag{C22}$$

From reference 20 (p. 35),

$$\int_0^\infty \exp(-\lambda t) J_0(2\beta t^{1/2}) dt = \frac{1}{\lambda} \exp\left(\frac{-\beta^2}{\lambda} \right) \tag{C23}$$

Combining equations (C22) and (C23) gives

$$H = \frac{4}{\frac{\mu^2}{4} + K^2 - \kappa^2 - i\mu\kappa} \int_0^\infty u^{-in} \exp\left(- \frac{\frac{\mu^2}{4} + K^2 + \kappa^2 - 2K\kappa \cos\theta}{\frac{\mu^2}{4} + K^2 - \kappa^2 - i\mu\kappa} u \right) du \tag{C24}$$

Integration with respect to u gives

$$H = 4\Gamma(1 - in) \frac{\left(\frac{\mu^2}{4} + K^2 - \kappa^2 - i\mu\kappa \right)^{-in}}{\left(\frac{\mu^2}{4} + K^2 + \kappa^2 - 2K\kappa \cos\theta \right)^{1-in}} \tag{C25}$$

With n treated as a constant, equation (C25) is substituted into equation (C21). The first and second derivatives of equation (C25) are taken, and then the result is simplified by substituting $n \equiv 1/\kappa a_0$ into the equation. Thus,

$$I_\kappa \, d\kappa \, d\sigma \, d\omega = \frac{128\pi^3}{h^4 a_0^4} \frac{e^4 m_e^2}{K^4} \frac{\kappa}{\left[1 - \exp\left(- \frac{2\pi}{\kappa a_0}\right)\right]} \frac{k'}{k} F \, d\kappa \, d\sigma \, d\omega \tag{C26}$$

where

$$F \equiv \frac{\mu^2 K^2 \left(C_0 + C_1 \cos\theta + C_2 \cos^2\theta + C_3 \cos^3\theta + C_4 \cos^4\theta\right)}{\left\{\left[\frac{\mu^2}{4} + (K+\kappa)^2\right]\left[\frac{\mu^2}{4} + (K-\kappa)^2\right]\right\}^2 \left(\frac{\mu^2}{4} + K^2 + \kappa^2 - 2K\kappa \cos\theta\right)^6} \exp\left(- \frac{2\mu}{\kappa} \arctan \frac{\mu\kappa}{\frac{\mu^2}{4} + K^2 - \kappa^2}\right) \tag{C27}$$

where

$$C_0 \equiv A_0^2 + B_0^2$$

$$C_1 \equiv 2(A_0 A_1 + B_0 B_1)$$

$$C_2 \equiv A_1^2 + B_1^2 + 2(A_0 A_2 + B_0 B_2)$$

$$C_3 \equiv 2(A_1 A_2 + B_1 B_2)$$

$$C_4 \equiv A_2^2 + B_2^2$$

$$A_0 \equiv - \frac{\mu^4 K}{8} + 2\mu^2 K\kappa^2 + 3\mu^2 K^3 - 2K^5 + 2K\kappa^4$$

$$A_1 \equiv \frac{7}{8} \mu^4 \kappa - \mu^2 \kappa^3 - 7\mu^2 K^2 \kappa - 4K^2 \kappa^3 + 6K^4 \kappa - 2\kappa^5$$

$$A_2 \equiv -\mu^4 K + 3\mu^2 K\kappa^2 - 4K^3 \kappa^2 + 4K\kappa^4$$

$$B_0 \equiv \mu^3 K\kappa$$

$$B_1 \equiv \frac{\mu^5}{8} - 3\mu^3 K^2 - 2\mu^3\kappa^2 + 2\mu K^4 - 2\mu\kappa^4$$

$$B_2 \equiv 4\mu^3 K\kappa - 4\mu K^3\kappa + 4\mu K\kappa^3$$

The solid angle $d\omega$ is given by

$$d\omega = 2\pi \sin\theta \, d\theta \tag{C28}$$

Substitution of equations (C27) and (C28) into equation (C26) gives

$$d\kappa \, d\sigma \int I_\kappa \, d\omega = \frac{2^8\pi^4 m_e^2 e^4}{h^4 a_0^6\left[1 - \exp\left(-\frac{2\pi}{\kappa a_0}\right)\right]} \frac{k'\kappa}{kK^2} \frac{\exp\left(-\frac{2\mu}{\kappa}\arctan\frac{\mu\kappa}{\frac{\mu^2}{4} + K^2 - \kappa^2}\right)}{\left\{\left[\frac{\mu^2}{4} + (K+\kappa)^2\right]\left[\frac{\mu^2}{4} + (K-\kappa)^2\right]\right\}^2} d\kappa \, d\sigma$$

$$\times \int_{-1}^{1} \frac{\left(C_0 + C_1 x + C_2 x^2 + C_3 x^3 + C_4 x^4\right)dx}{\left(\frac{\mu^2}{4} + K^2 + \kappa^2 - 2K\kappa x\right)^6} \tag{C29}$$

where

$$x \equiv \cos\theta \tag{C30}$$

If

$$a \equiv \frac{\mu^2}{4} + K^2 + \kappa^2 \tag{C31}$$

and

$$b \equiv -2K\kappa \tag{C32}$$

the integral in equation (C29) becomes

$$I = -\frac{1}{5b}\left[\frac{1}{(a+b)^5} - \frac{1}{(a-b)^5}\right]\left(C_0 - C_1\frac{a}{b} + C_2\frac{a^2}{b^2} - C_3\frac{b}{a}\right) + \frac{C_4}{5a}\left[\frac{1}{(a+b)^5} + \frac{1}{(a-b)^5}\right]$$

$$-\frac{1}{4b^2}\left[\frac{1}{(a+b)^4} - \frac{1}{(a-b)^4}\right]\left(C_1 - 2C_2\frac{a}{b} - C_3\frac{b^2}{5a^2}\right) - \frac{C_2}{3b^3}\left[\frac{1}{(a+b)^3} - \frac{1}{(a-b)^3}\right] \tag{C33}$$

The solid angle $d\sigma$ is given by

$$d\sigma = 2\pi \sin\delta\, d\delta \tag{C34}$$

Making use of the differential form of equation (C7) yields

$$d\sigma = 2\pi \frac{K\, dK}{kk'} \tag{C35}$$

The Bohr radius,

$$a_0 = \frac{h^2}{4\pi^2 m_e e^2} \tag{C36}$$

and equations (C33) and (C35) are substituted into equation (C29) to get

$$Q_{ion} = \frac{2^5\pi}{k^2 a_0^8}\int_0^{\kappa_{max}} \frac{\kappa\, d\kappa}{\left[1 - \exp\left(\frac{-2\pi}{\kappa a_0}\right)\right]}\int_{K_{min}}^{K_{max}} \frac{I \exp\left(-\frac{2\mu}{\kappa}\arctan\frac{\mu\kappa}{\frac{\mu^2}{4} + K^2 - \kappa^2}\right)}{\left\{\left[\frac{\mu^2}{4} + (K+\kappa)^2\right]\left[\frac{\mu^2}{4} + (K-\kappa)^2\right]\right\}^2}\frac{dK}{K} \tag{C37}$$

where

$$K_{max} \equiv k + k' \tag{C38}$$

$$K_{min} \equiv k - k' \tag{C39}$$

$$k' \equiv \sqrt{k^2 - \kappa^2 - \frac{8\pi^2 m_e}{h^2} U_i} \tag{C40}$$

$$\kappa_{max} \equiv \sqrt{k^2 - \frac{8\pi^2 m_e}{h^2} U_i} \tag{C41}$$

and U_i is the energy of ionization. The term Q_{ion} represents the total ionization cross section from the 2s level. This form is the one which Mandl (ref. 14) uses. Others (refs. 11, 13, and 15) go further and make the substitutions required in equation (C33). The results of these substitutions agree with those of Burhop (ref. 11) and are as follows:

$$I(K, \kappa)dK\, d\kappa = \frac{2^8 \pi \kappa}{15k^2 K a_0^8} \frac{\exp\left(-\frac{2\mu}{\kappa} \arctan \frac{\mu\kappa}{\frac{\mu^2}{4} + K^2 - \kappa^2}\right) A\, dK\, d\kappa}{\left[1 - \exp\left(-\frac{2\pi}{\kappa a_0}\right)\right]\left\{\left[\frac{\mu^2}{4} + (K + \kappa)^2\right]\left[\frac{\mu^2}{4} + (K - \kappa)^2\right]\right\}^5} \tag{18}$$

where

$$A \equiv \frac{5}{256} \mu^{10} + \frac{\mu^8}{256} (47K^2 + 85\kappa^2) + \frac{\mu^6}{16} (25K^4 + 35\kappa^4)$$

$$+ \frac{\mu^4}{8} (205K^6 - 155K^4\kappa^2 - 41K^2\kappa^4 + 55\kappa^6)$$

$$- 10\mu^2\left(K^2 - \kappa^2\right)^2 (4K^4 - K^2\kappa^2 - \kappa^4) + 5\left(K^2 - \kappa^2\right)^4 (3K^2 + \kappa^2) \tag{19}$$

REFERENCES

1. Stebbings, R. F.; Fite, Wade L.; Hummer, David G.; and Brackmann, R. T.: Collisions of Electrons with Hydrogen Atoms. V. Excitation of Metastable 2s Hydrogen Atoms. Phys. Rev., vol. 119, no. 6, Sept. 15, 1960, pp. 1939-1945.

2. Fite, Wade L.; and Brackmann, R. T.: Collisions of Electrons with Hydrogen Atoms. II. Excitation of Lyman-Alpha Radiation. Phys. Rev., vol. 112, no. 4, Nov. 15, 1958, pp. 1151-1156.,

3. Omidvar, Kazem: 2s and 2p Electron Impact Excitation in Atomic Hydrogen. Phys. Rev., vol. 133, no. 4A, Feb. 17, 1964, pp. 970-985.

4. Saraph, H. E.: Cross Sections for $n \rightarrow n + 1$ Transitions in Hydrogen Produced by Electron Impact. Proc. Phys. Soc., vol. 83, May 1964, pp. 763-768.

5. Kingston, A. E.: Excitation and Ionization of Hydrogen Atoms by Electron Impact. Phys. Rev., vol. 135, no. 6A, Sept. 14, 1964, pp. 1529-1536.

6. McCarroll, R.: The Excitation of the Discrete Levels of Atomic Hydrogen by Fast Electrons. Proc. Phys. Soc., ser. A, vol. 70, pt. 6, June 1957, pp. 460-465.

7. Ochkur, V. I.; and Petrunkin, A. M.: The Classical Calculation of the Probabilities of Excitation and Ionization of Atoms by Electron Impact. Optics and Spectroscopy, vol. 14, no. 3, Mar. 1963, pp. 245-248.

8. Massey, H. S. W.; and Mohr, C. B. O.: The Collision of Electrons with Simple Atomic Systems and Electron Exchange. Proc. Roy. Soc. (London), ser. A, vol. 132, no. 820, Aug. 1, 1931, pp. 605-630.

9. Massey, H. S. W.; and Mohr, C. B. O.: The Collision of Slow Electrons with Atoms. III. The Excitation and Ionization of Helium by Electrons of Moderate Velocity. Roy. Soc. Proc., ser. A, vol. 140, no. 842, June 1, 1933, pp. 613-636.

10. Monnin, Carl F.; and Prok, George M.: Comparison of Gryzinski's and Born's Approximations for Inelastic Scattering in Atomic Hydrogen. NASA TN D-2903, 1965.

11. Burhop, E. H. S.: The Inner Shell Ionization of Atoms by Electron Impact. Proc. Cambridge Phil. Soc. Proc., vol. 36, pt. 1, Jan. 1940, pp. 43-52.

12. Boyd, T. J. M.: Electron Excitation of Atomic Hydrogen in the 2s State. Phys. Soc. Proc., vol. 72, pt. 4, Oct. 1958, pp. 523-531.

13. Swan, P.: The Ionization by Electrons of the Excited 2s and 2p States of Atomic Hydrogen. Phys. Soc. Proc., vol. 68, pt. 12, Dec. 1955, pp. 1157-1160.

14. Mandl, F.: The Ionization by Electron Impact of Excited Hydrogen Atoms. AEC Rep. No. A.E.R.E. T/R. 1006, 1952.

15. Sellin, I. A.: Experiments on the Production and Extinction of the 2s State of the Hydrogen Atom. Phys. Rev., vol. 136, no. 5A, Nov. 30, 1964, pp. A1245-1253.

16. Fite, Wade L.; Brackmann, R. T.; Hummer, David G.; and Stebbings, R. F.: Lifetime of the 2s State of Atomic Hydrogen. Phys. Rev., vol. 116, no. 2, Oct. 15, 1959, pp. 363-367.

17. Gryzinski, Michal: Classical Theory of Atomic Collisions. I. Theory of Inelastic Collisions. Phys. Rev., vol. 138, no. 2A, Apr. 19, 1965, pp. 336-358.

18. Gryzinski, Michal: Classical Theory of Electronic and Ionic Inelastic Collisions. Phys. Rev., vol. 115, no. 2, July 15, 1959, pp. 374-383.

19. Schiff, L. I.: Quantum Mechanics. Second ed., McGraw-Hill Book Co., Inc., 1955.

20. Magnus, W.; and Oberhettinger, F. (J. Werner, trans.): Formulas and Theorems for the Functions of Mathematical Physics. Chelsea Pub. Co., Inc., 1949.

21. Morse, P. M.; and Feshbach, H.: Methods of Theoretical Physics. McGraw-Hill Book Co., Inc., 1953.

22. Watson, G. N.: A Treatise on the Theory of Bessel Functions. 2nd ed., Univ. Press, Cambridge, England; Macmillan Co., New York, 1944.

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